



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:37 PM UTC

PDB ID : 2V4M / pdb_00002v4m
Title : The isomerase domain of human glutamine-fructose-6-phosphate transaminase 1 (GFPT1) in complex with fructose 6-phosphate
Authors : Moche, M.; Lehtio, L.; Andersson, J.; Arrowsmith, C.H.; Berglund, H.; Collins, R.; Dahlgren, L.G.; Edwards, A.M.; Flodin, S.; Flores, A.; Graslund, S.; Hammarstrom, M.; Johansson, A.; Johansson, I.; Karlberg, T.; Kotenyova, T.; Nilsson, M.E.; Nyman, T.; Persson, C.; Sagemark, J.; Svensson, S.; Schueler, H.; Thorsell, A.G.; Tresaugues, L.; Uppenberg, J.; Van Den Berg, S.; Welin, M.; Wisniewska, M.; Weigelt, J.; Nordlund, P.; Wikstrom, M.
Deposited on : 2008-09-26
Resolution : 2.29 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	: 4-5-2 with Phenix2.0
Mogul	: 2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	: 2.0
EDS	: 3.0
Buster-report	: wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	: 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	: 9.0.010 (Gargrove)

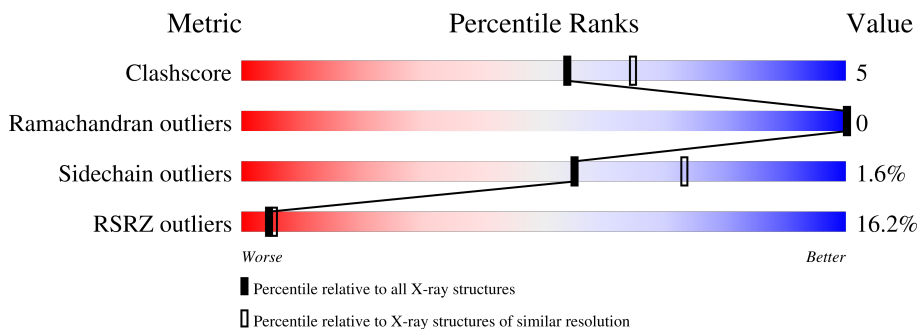
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	376	15% 84% 9% 6%
1	B	376	38% 77% 16% 7%
1	C	376	4% 84% 10% 6%
1	D	376	3% 83% 10% 7%

Density-Fitness : 1.0.12
 Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

2 Entry composition [i](#)

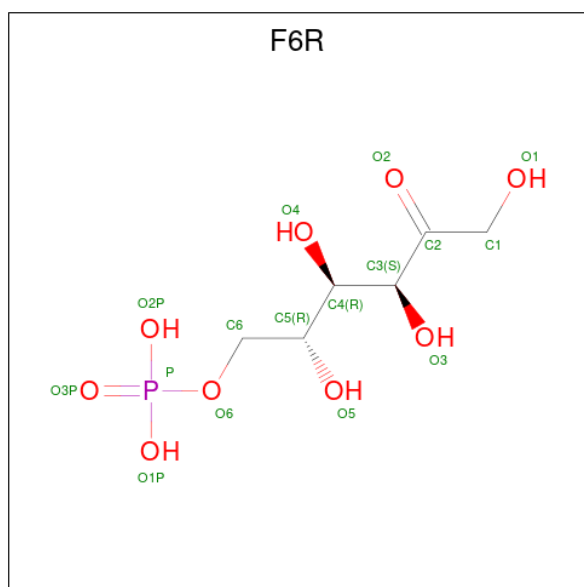
There are 4 unique types of molecules in this entry. The entry contains 11333 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called GLUCOSAMINE--FRUCTOSE-6-PHOSPHATE AMINO-TRANSFERASE [ISOMERIZING] 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	352	Total	C	N	O	S	0	3	0
			2775	1747	482	518	28			
1	B	351	Total	C	N	O	S	0	2	0
			2762	1739	481	516	26			
1	C	352	Total	C	N	O	S	0	4	0
			2794	1760	488	519	27			
1	D	350	Total	C	N	O	S	0	4	0
			2773	1745	483	518	27			

- Molecule 2 is FRUCTOSE -6-PHOSPHATE (CCD ID: F6R) (formula: C₆H₁₃O₉P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			16	6	9	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	O	P	0	0
			16	6	9	1		
2	C	1	Total	C	O	P	0	0
			16	6	9	1		
2	D	1	Total	C	O	P	0	0
			16	6	9	1		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	Cl	0	0
			1	1		

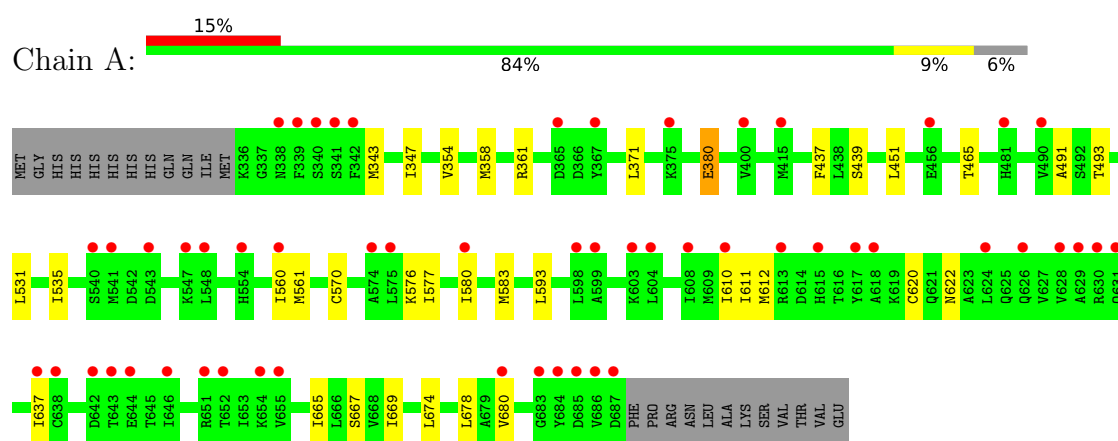
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	35	Total	O	0	0
			35	35		
4	B	14	Total	O	0	0
			14	14		
4	C	50	Total	O	0	0
			50	50		
4	D	65	Total	O	0	0
			65	65		

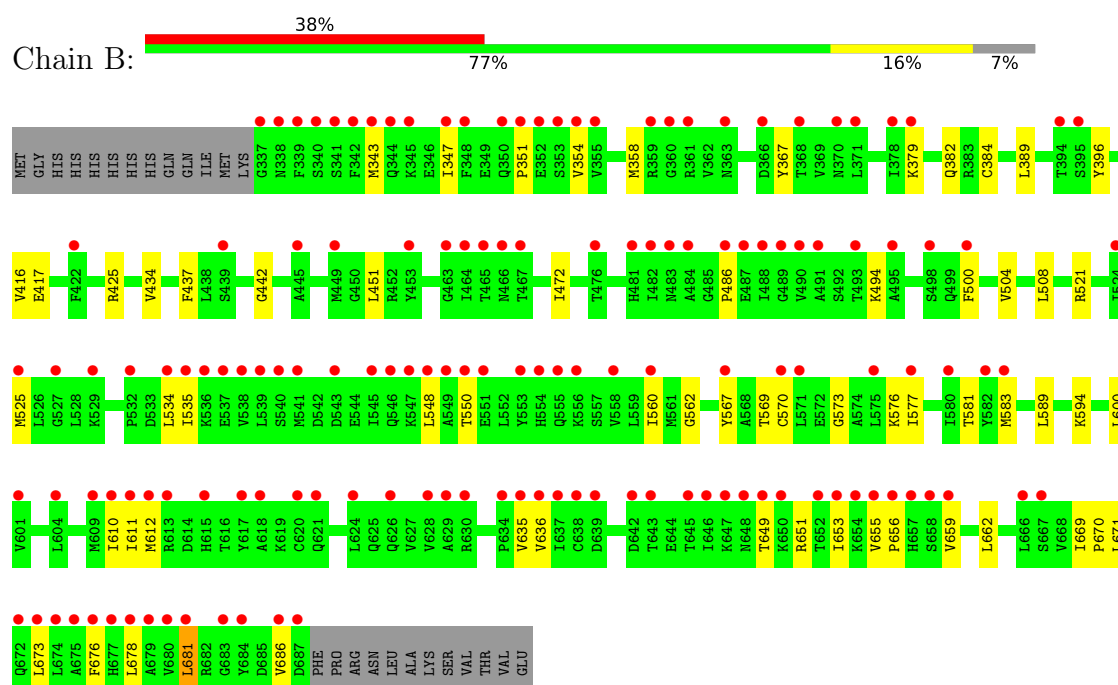
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: GLUCOSAMINE--FRUCTOSE-6-PHOSPHATE AMINOTRANSFERASE [ISOMERIZING] 1

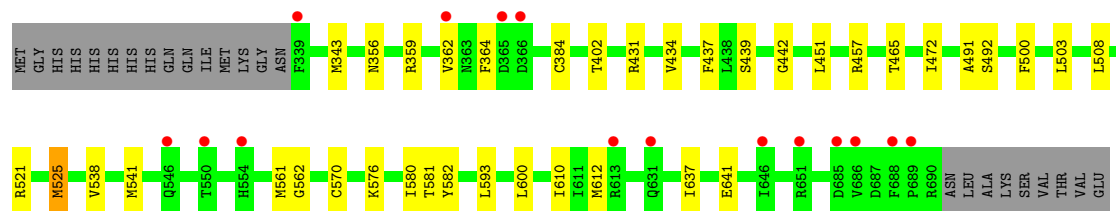


• Molecule 1: GLUCOSAMINE--FRUCTOSE-6-PHOSPHATE AMINOTRANSFERASE [ISOMERIZING] 1



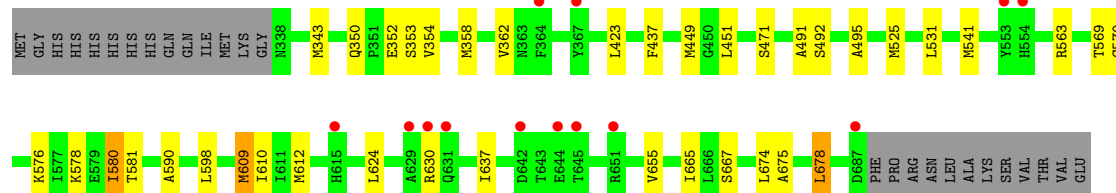
● Molecule 1: GLUCOSAMINE--FRUCTOSE-6-PHOSPHATE AMINOTRANSFERASE [ISOMERIZING] 1

Chain C: 



● Molecule 1: GLUCOSAMINE--FRUCTOSE-6-PHOSPHATE AMINOTRANSFERASE [ISOMERIZING] 1

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	178.82Å 178.82Å 157.11Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	54.89 – 2.29 54.89 – 2.29	Depositor EDS
% Data completeness (in resolution range)	99.2 (54.89-2.29) 97.0 (54.89-2.29)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.17 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0035	Depositor
R, R_{free}	0.167 , 0.185 0.221 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	40.7	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 32.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	0.000 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.679 for H, K, L 0.321 for -H-K, K, -L	Depositor
Outliers	0 of 81887 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11333	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: F6R, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.54	0/2815	0.73	0/3794
1	B	0.51	0/2803	0.73	0/3780
1	C	0.59	0/2836	0.76	0/3824
1	D	0.63	0/2813	0.74	0/3792
All	All	0.57	0/11267	0.74	0/15190

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2775	0	2833	24	0
1	B	2762	0	2814	42	0
1	C	2794	0	2849	22	0
1	D	2773	0	2829	25	0
2	A	16	0	11	0	0
2	B	16	0	11	1	0
2	C	16	0	11	0	0
2	D	16	0	11	0	0
3	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	35	0	0	0	0
4	B	14	0	0	0	0
4	C	50	0	0	0	0
4	D	65	0	0	0	0
All	All	11333	0	11369	111	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (111) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:563:ARG:HG3	1:D:590:ALA:HB3	1.40	1.01
1:B:343:MET:HE2	1:B:347:ILE:HD11	1.47	0.95
1:B:548:LEU:HD22	1:B:653:ILE:HD11	1.63	0.81
1:D:612:MET:HE1	1:D:637:ILE:HG22	1.67	0.77
1:D:612:MET:CE	1:D:637:ILE:HG22	2.17	0.74
1:D:491:ALA:HB1	1:D:576:LYS:HE3	1.71	0.73
1:C:508:LEU:O	1:C:521[A]:ARG:NH1	2.23	0.71
1:D:423:LEU:HD13	1:D:449[B]:MET:HE2	1.76	0.67
1:B:576:LYS:NZ	2:B:800:F6R:O1	2.23	0.67
1:B:550:THR:HG22	1:B:681:LEU:HD21	1.76	0.67
1:C:362:VAL:HG13	1:C:525:MET:HE1	1.79	0.64
1:D:362:VAL:HG13	1:D:525:MET:HE3	1.80	0.64
1:A:570[B]:CYS:SG	1:A:610:ILE:HD12	2.38	0.63
1:B:389:LEU:HD12	1:B:416:VAL:HG22	1.81	0.62
1:D:570[B]:CYS:SG	1:D:610:ILE:HD12	2.42	0.60
1:B:396:TYR:CE1	1:B:416:VAL:HG12	2.37	0.60
1:A:611:ILE:HD12	1:A:620:CYS:HB3	1.85	0.59
1:B:384:CYS:SG	1:B:434:VAL:HG23	2.43	0.59
1:D:354:VAL:HG12	1:D:358:MET:HE2	1.85	0.58
1:B:417:GLU:OE1	1:B:425:ARG:NH2	2.35	0.58
1:B:569:THR:HG21	1:B:610:ILE:HD13	1.85	0.58
1:D:354:VAL:CG1	1:D:358:MET:HE2	2.34	0.57
1:C:612:MET:HE1	1:C:637:ILE:HG22	1.89	0.55
1:B:354:VAL:HG12	1:B:358:MET:HE2	1.88	0.54
1:D:343:MET:SD	1:D:580:ILE:HD13	2.47	0.54
1:B:548:LEU:HD21	1:B:635:VAL:HG11	1.89	0.54
1:C:491:ALA:HB1	1:C:576:LYS:HE3	1.90	0.54
1:B:573:GLY:HA3	1:B:671:LEU:HD13	1.91	0.53
1:B:486:PRO:O	1:B:494:LYS:NZ	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:655:VAL:HG13	1:B:656:PRO:HD2	1.91	0.52
1:C:362:VAL:HG13	1:C:525:MET:CE	2.40	0.52
1:B:659:VAL:HG12	1:B:662:LEU:HD12	1.91	0.52
1:D:598:LEU:O	1:D:630:ARG:NH1	2.42	0.52
1:A:354:VAL:CG1	1:A:358:MET:HE2	2.40	0.52
1:B:569:THR:CG2	1:B:610:ILE:HD13	2.39	0.52
1:B:611:ILE:HD12	1:B:636:VAL:HG13	1.92	0.52
1:D:343:MET:HE1	1:D:580:ILE:HD13	1.92	0.52
1:C:538:VAL:HA	1:C:541:MET:HE3	1.92	0.51
1:C:570[B]:CYS:SG	1:C:610:ILE:HD12	2.51	0.51
1:A:531:LEU:HD21	1:A:665:ILE:HD13	1.93	0.51
1:B:442:GLY:HA2	1:B:472:ILE:HD12	1.93	0.51
1:A:437:PHE:CZ	1:A:451:LEU:HA	2.46	0.50
1:C:561:MET:SD	1:C:593:LEU:HD11	2.51	0.50
1:D:541:MET:HE1	1:D:655:VAL:HA	1.93	0.50
1:C:362:VAL:HG11	1:C:364:PHE:CE1	2.47	0.50
1:B:635:VAL:HG22	1:B:651:ARG:HD2	1.94	0.50
1:A:583:MET:HE1	1:A:678:LEU:HD21	1.94	0.49
1:A:361:ARG:HG2	1:A:371:LEU:HD23	1.93	0.49
1:A:583:MET:CE	1:A:678:LEU:HD21	2.43	0.49
1:A:560:ILE:HD11	1:A:577:ILE:HD12	1.95	0.49
1:A:612:MET:HE1	1:A:637:ILE:HG22	1.94	0.49
1:A:354:VAL:HG12	1:A:358:MET:HE2	1.95	0.48
1:C:437:PHE:CZ	1:C:451:LEU:HA	2.49	0.48
1:C:356:ASN:OD1	1:C:359:ARG:NH1	2.46	0.48
1:B:567:TYR:CD1	1:B:589:LEU:HD13	2.49	0.48
1:D:569:THR:HG21	1:D:667[A]:SER:OG	2.14	0.48
1:B:611:ILE:HD12	1:B:636:VAL:CG1	2.44	0.48
1:C:439:SER:O	1:C:465:THR:HA	2.14	0.48
1:D:437:PHE:CZ	1:D:451:LEU:HA	2.48	0.47
1:D:531:LEU:HD21	1:D:665:ILE:HD13	1.95	0.47
1:B:583:MET:HE1	1:B:678:LEU:HD13	1.96	0.47
1:B:562:GLY:HA3	1:B:570[B]:CYS:SG	2.54	0.47
1:A:610:ILE:O	1:A:611:ILE:HD13	2.15	0.47
1:C:612:MET:CE	1:C:637:ILE:HG22	2.44	0.47
1:D:674:LEU:HG	1:D:678:LEU:HD22	1.97	0.46
1:A:535:ILE:HG23	1:A:669:ILE:CD1	2.45	0.46
1:B:379:LYS:HA	1:B:382:GLN:HE21	1.81	0.46
1:B:367:TYR:HB3	1:B:525:MET:HE1	1.96	0.46
1:B:550:THR:CG2	1:B:681:LEU:HD11	2.46	0.46
1:B:508:LEU:HD22	1:B:521:ARG:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:550:THR:HG22	1:B:681:LEU:HD11	1.99	0.45
1:B:534:LEU:HD22	1:B:656:PRO:HB2	1.99	0.45
1:B:351:PRO:HG3	1:B:535:ILE:HG22	1.99	0.45
1:C:343:MET:HE1	1:C:580:ILE:HD13	1.98	0.45
1:B:347:ILE:HG21	1:B:673:LEU:CD2	2.47	0.44
1:B:437:PHE:CZ	1:B:451:LEU:HA	2.51	0.44
1:A:674:LEU:O	1:A:678:LEU:HB2	2.17	0.44
1:D:609:MET:HB2	1:D:609:MET:HE2	1.75	0.44
1:A:491:ALA:HB1	1:A:576:LYS:HE3	1.99	0.44
1:B:500:PHE:O	1:B:504:VAL:HG23	2.17	0.44
1:A:439:SER:O	1:A:465:THR:HA	2.18	0.43
1:A:535:ILE:HG23	1:A:669:ILE:HD13	2.00	0.43
1:D:492:SER:OG	1:D:495:ALA:HB3	2.18	0.43
1:A:343:MET:SD	1:A:580:ILE:HD13	2.59	0.43
1:C:442:GLY:C	1:C:472:ILE:HD12	2.43	0.43
1:A:380:GLU:HG2	1:C:431:ARG:HD2	2.00	0.43
1:D:354:VAL:HG12	1:D:358:MET:CE	2.48	0.42
1:B:548:LEU:CD2	1:B:653:ILE:HD11	2.43	0.42
1:C:562:GLY:N	1:C:570[B]:CYS:SG	2.92	0.42
1:D:350:GLN:HA	1:D:353:SER:OG	2.19	0.42
1:B:636:VAL:HG23	1:B:649:THR:HG21	2.02	0.42
1:A:612:MET:CE	1:A:637:ILE:HG22	2.50	0.42
1:A:347:ILE:HG13	1:A:493:THR:HG21	2.02	0.42
1:D:580:ILE:HD11	1:D:675:ALA:C	2.45	0.42
1:A:612:MET:HE3	1:A:667:SER:CB	2.50	0.41
1:A:561:MET:HE2	1:A:593:LEU:HD21	2.03	0.41
1:B:384:CYS:SG	1:B:434:VAL:CG2	3.07	0.41
1:C:402:THR:HG21	1:C:503:LEU:HB2	2.03	0.41
1:B:577:ILE:CG2	1:B:583:MET:HE3	2.51	0.41
1:B:560:ILE:HG22	1:B:570[B]:CYS:SG	2.61	0.41
1:B:577:ILE:HG21	1:B:583:MET:HE3	2.02	0.41
1:C:384[A]:CYS:CB	1:C:434:VAL:HG23	2.50	0.41
1:C:492:SER:O	1:C:576:LYS:HE2	2.21	0.41
1:A:531:LEU:HD21	1:A:665:ILE:CD1	2.51	0.40
1:B:569:THR:CG2	1:B:610:ILE:CD1	2.99	0.40
1:D:609:MET:HE3	1:D:624:LEU:HD13	2.03	0.40
1:B:669:ILE:HB	1:B:670:PRO:HD3	2.04	0.40
1:B:676:PHE:CD1	1:B:686:VAL:HG21	2.56	0.40
1:C:538:VAL:O	1:C:541:MET:HG2	2.21	0.40
1:D:423:LEU:HD11	1:D:449[B]:MET:HB2	2.04	0.40
1:C:600:LEU:HD22	1:D:578:LYS:HG2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	353/376 (94%)	342 (97%)	11 (3%)	0	100	100
1	B	351/376 (93%)	344 (98%)	7 (2%)	0	100	100
1	C	354/376 (94%)	349 (99%)	5 (1%)	0	100	100
1	D	352/376 (94%)	346 (98%)	6 (2%)	0	100	100
All	All	1410/1504 (94%)	1381 (98%)	29 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	311/330 (94%)	308 (99%)	3 (1%)	68	82
1	B	309/330 (94%)	304 (98%)	5 (2%)	55	73
1	C	313/330 (95%)	307 (98%)	6 (2%)	50	69
1	D	311/330 (94%)	305 (98%)	6 (2%)	50	69
All	All	1244/1320 (94%)	1224 (98%)	20 (2%)	55	73

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	380	GLU
1	A	622	ASN
1	A	680	VAL
1	B	581	THR
1	B	594	LYS
1	B	600	LEU
1	B	612	MET
1	B	681	LEU
1	C	457	ARG
1	C	500	PHE
1	C	525	MET
1	C	581	THR
1	C	582	TYR
1	C	641	GLU
1	D	352	GLU
1	D	471	SER
1	D	580	ILE
1	D	581	THR
1	D	609	MET
1	D	678	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	344	GLN
1	A	370	ASN
1	A	622	ASN
1	B	382	GLN
1	B	404	GLN
1	B	426	ASN
1	C	546	GLN
1	D	440	GLN
1	D	466	ASN
1	D	499	GLN
1	D	626	GLN
1	D	657	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	F6R	D	800	-	15,15,15	0.68	0	16,21,21	1.08	1 (6%)
2	F6R	A	800	-	15,15,15	0.63	0	16,21,21	0.82	0
2	F6R	C	800	-	15,15,15	0.55	0	16,21,21	1.09	0
2	F6R	B	800	-	15,15,15	0.51	0	16,21,21	0.92	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	F6R	D	800	-	-	0/20/20/20	-
2	F6R	A	800	-	-	0/20/20/20	-
2	F6R	C	800	-	-	0/20/20/20	-
2	F6R	B	800	-	-	0/20/20/20	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	800	F6R	O1P-P-O6	-2.16	101.03	106.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	800	F6R	C5-C4-C3	-2.01	108.74	112.05

There are no chirality outliers.

There are no torsion outliers.

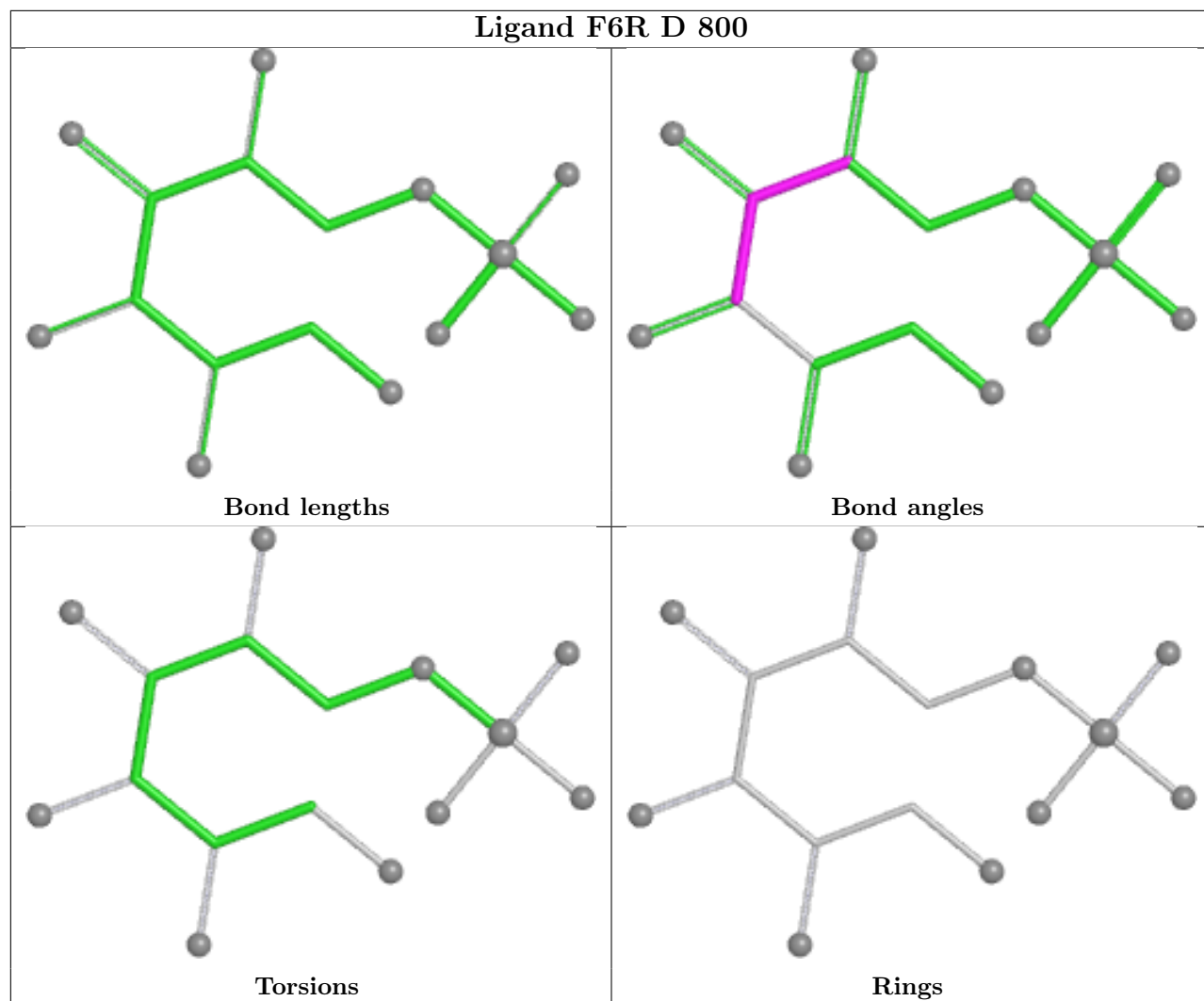
There are no ring outliers.

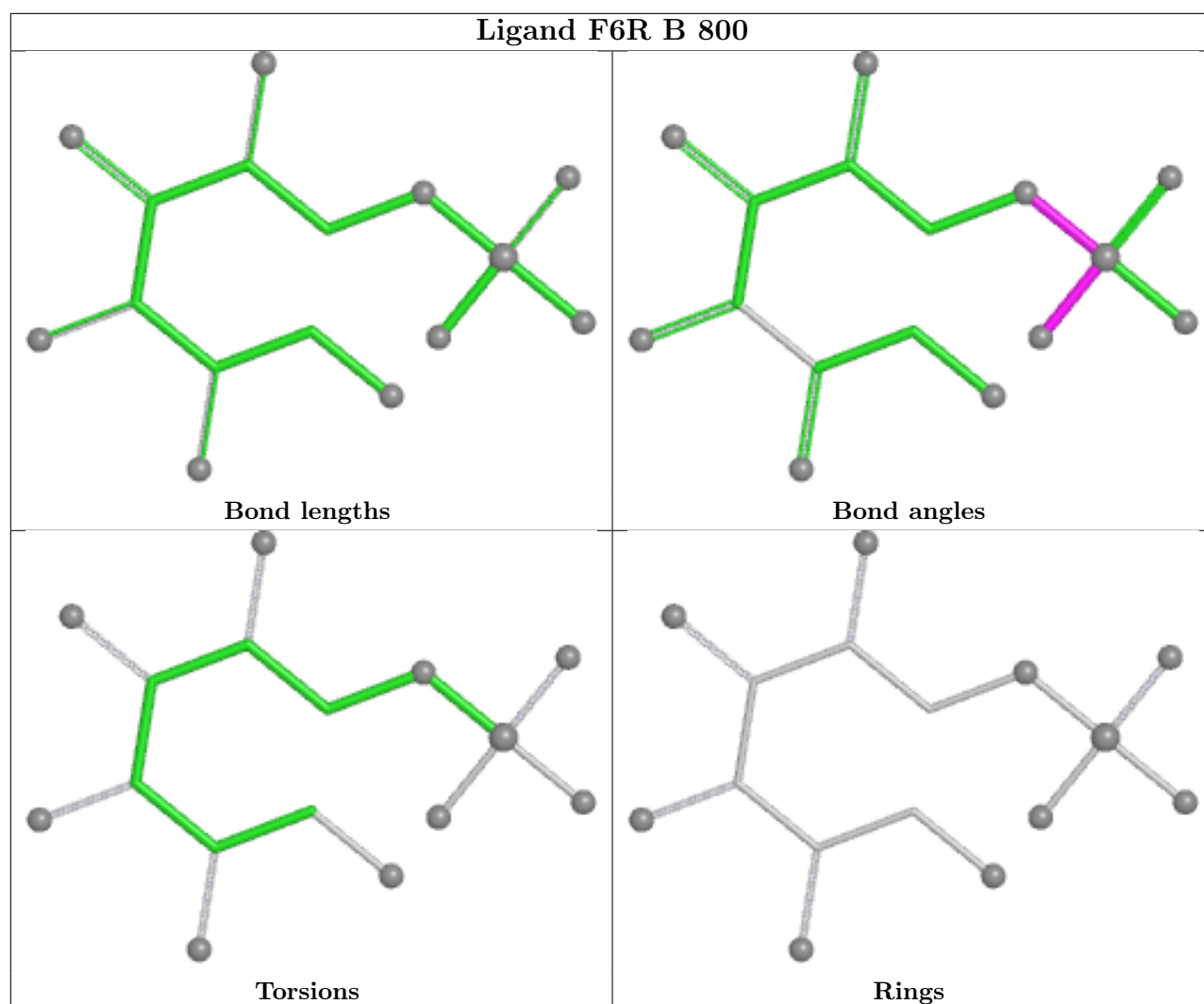
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	800	F6R	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand F6R D 800





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	352/376 (93%)	0.99	55 (15%) 5 6	17, 44, 69, 76	3 (0%)
1	B	351/376 (93%)	1.78	144 (41%) 0 0	26, 59, 79, 85	2 (0%)
1	C	352/376 (93%)	0.56	15 (4%) 40 41	15, 37, 58, 66	4 (1%)
1	D	350/376 (93%)	0.36	13 (3%) 45 48	13, 33, 51, 55	4 (1%)
All	All	1405/1504 (93%)	0.93	227 (16%) 4 5	13, 41, 73, 85	13 (0%)

All (227) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	489	GLY	5.6
1	B	490	VAL	5.1
1	B	680	VAL	4.7
1	A	684	TYR	4.6
1	B	337	GLY	4.6
1	B	617	TYR	4.4
1	B	341	SER	4.3
1	C	689	PRO	4.2
1	A	613	ARG	4.1
1	D	642	ASP	4.1
1	B	532	PRO	4.1
1	B	642	ASP	4.1
1	B	687	ASP	4.0
1	A	339	PHE	4.0
1	A	680	VAL	4.0
1	C	688	PHE	3.9
1	A	628	VAL	3.9
1	B	355	VAL	3.9
1	B	352	GLU	3.8
1	B	339	PHE	3.8
1	A	683	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	347	ILE	3.7
1	B	545	ILE	3.7
1	B	340	SER	3.7
1	A	608	ILE	3.6
1	B	686	VAL	3.6
1	B	637	ILE	3.6
1	B	342	PHE	3.6
1	B	615[A]	HIS	3.6
1	B	495	ALA	3.6
1	B	539	LEU	3.6
1	D	631	GLN	3.5
1	B	536	LYS	3.5
1	B	538	VAL	3.5
1	B	549	ALA	3.4
1	B	482	ILE	3.4
1	B	580	ILE	3.4
1	B	488	ILE	3.4
1	B	646	ILE	3.4
1	B	649	THR	3.4
1	C	366	ASP	3.4
1	A	490	VAL	3.3
1	B	338	ASN	3.3
1	B	353	SER	3.3
1	A	637	ILE	3.3
1	B	535	ILE	3.3
1	A	367	TYR	3.3
1	A	629	ALA	3.2
1	B	439	SER	3.2
1	A	651	ARG	3.2
1	B	657	HIS	3.2
1	A	685	ASP	3.2
1	B	676	PHE	3.1
1	B	679	ALA	3.1
1	C	686	VAL	3.1
1	A	604	LEU	3.1
1	A	375	LYS	3.1
1	B	645	THR	3.1
1	B	348	PHE	3.1
1	B	543	ASP	3.1
1	B	653	ILE	3.1
1	D	615	HIS	3.1
1	B	658	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	360	GLY	3.1
1	B	351	PRO	3.1
1	B	656	PRO	3.1
1	B	673	LEU	3.1
1	A	610	ILE	3.0
1	B	463	GLY	3.0
1	B	674	LEU	3.0
1	A	560	ILE	3.0
1	B	548	LEU	3.0
1	B	659	VAL	3.0
1	B	524	ILE	3.0
1	B	611	ILE	3.0
1	A	615	HIS	2.9
1	A	646	ILE	2.9
1	A	624	LEU	2.9
1	B	675	ALA	2.9
1	B	582	TYR	2.8
1	A	655	VAL	2.8
1	B	493	THR	2.8
1	A	687	ASP	2.8
1	A	341	SER	2.8
1	B	361	ARG	2.8
1	B	678	LEU	2.8
1	B	681	LEU	2.8
1	A	643	THR	2.8
1	B	484	ALA	2.8
1	B	638	CYS	2.8
1	B	635	VAL	2.8
1	B	476	THR	2.7
1	B	537	GLU	2.7
1	C	646	ILE	2.7
1	A	603	LYS	2.7
1	A	342	PHE	2.7
1	A	630	ARG	2.7
1	A	541	MET	2.7
1	B	654	LYS	2.6
1	A	540	SER	2.6
1	A	554	HIS	2.6
1	A	644	GLU	2.6
1	C	685	ASP	2.6
1	C	613	ARG	2.6
1	B	643	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	645	THR	2.6
1	B	629	ALA	2.6
1	B	394	THR	2.6
1	B	655	VAL	2.6
1	B	650	LYS	2.6
1	B	570[A]	CYS	2.6
1	A	599	ALA	2.6
1	B	550	THR	2.6
1	C	339	PHE	2.6
1	B	567	TYR	2.6
1	D	554	HIS	2.5
1	B	612	MET	2.5
1	B	628	VAL	2.5
1	D	644	GLU	2.5
1	A	338	ASN	2.5
1	B	626	GLN	2.5
1	B	540	SER	2.5
1	B	464	ILE	2.5
1	B	571	LEU	2.5
1	B	466	ASN	2.5
1	B	527	GLY	2.5
1	B	667	SER	2.4
1	B	525	MET	2.4
1	B	363	ASN	2.4
1	B	445	ALA	2.4
1	D	629	ALA	2.4
1	B	551	GLU	2.4
1	A	400	VAL	2.4
1	A	686	VAL	2.4
1	B	547	LYS	2.4
1	B	553	TYR	2.4
1	B	465	THR	2.4
1	B	577	ILE	2.4
1	B	609	MET	2.4
1	A	631	GLN	2.4
1	D	651	ARG	2.4
1	A	574	ALA	2.4
1	B	491	ALA	2.4
1	A	415[A]	MET	2.4
1	B	613	ARG	2.3
1	A	626	GLN	2.3
1	B	639	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	575	LEU	2.3
1	A	617	TYR	2.3
1	B	683	GLY	2.3
1	C	550	THR	2.3
1	A	340	SER	2.3
1	B	359	ARG	2.3
1	B	498	SER	2.3
1	B	621	GLN	2.3
1	B	672	GLN	2.3
1	B	647	LYS	2.3
1	C	365	ASP	2.3
1	B	453	TYR	2.3
1	B	554	HIS	2.3
1	C	554	HIS	2.3
1	B	344	GLN	2.3
1	A	575	LEU	2.2
1	B	449	MET	2.2
1	B	541	MET	2.2
1	A	456	GLU	2.2
1	A	652	THR	2.2
1	B	395	SER	2.2
1	B	379	LYS	2.2
1	B	422	PHE	2.2
1	B	601	VAL	2.2
1	B	483	ASN	2.2
1	D	687	ASP	2.2
1	B	620	CYS	2.2
1	A	580	ILE	2.2
1	A	642	ASP	2.2
1	B	648	ASN	2.2
1	B	546	GLN	2.2
1	A	548	LEU	2.2
1	B	560	ILE	2.2
1	B	604	LEU	2.2
1	B	610	ILE	2.2
1	B	558	VAL	2.2
1	B	345	LYS	2.2
1	C	631	GLN	2.2
1	B	618	ALA	2.2
1	A	543	ASP	2.1
1	B	467	THR	2.1
1	D	630	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	684	TYR	2.1
1	D	367	TYR	2.1
1	A	598	LEU	2.1
1	B	556	LYS	2.1
1	B	366	ASP	2.1
1	B	354	VAL	2.1
1	B	350	GLN	2.1
1	B	634	PRO	2.1
1	C	546	GLN	2.1
1	B	630	ARG	2.1
1	B	487	GLU	2.1
1	D	553	TYR	2.1
1	C	362	VAL	2.1
1	C	651	ARG	2.1
1	A	654	LYS	2.1
1	B	371	LEU	2.1
1	B	481	HIS	2.1
1	B	636	VAL	2.1
1	D	364	PHE	2.1
1	A	618	ALA	2.0
1	A	481	HIS	2.0
1	B	555	GLN	2.0
1	B	677	HIS	2.0
1	B	624	LEU	2.0
1	B	666	LEU	2.0
1	B	486	PRO	2.0
1	B	500	PHE	2.0
1	A	547	LYS	2.0
1	B	529	LYS	2.0
1	B	343	MET	2.0
1	B	583	MET	2.0
1	B	368	THR	2.0
1	B	652	THR	2.0
1	A	638	CYS	2.0
1	A	365	ASP	2.0
1	B	370	ASN	2.0
1	B	534	LEU	2.0
1	B	378	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

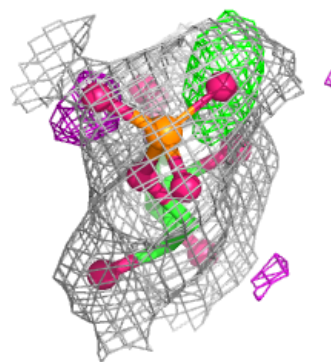
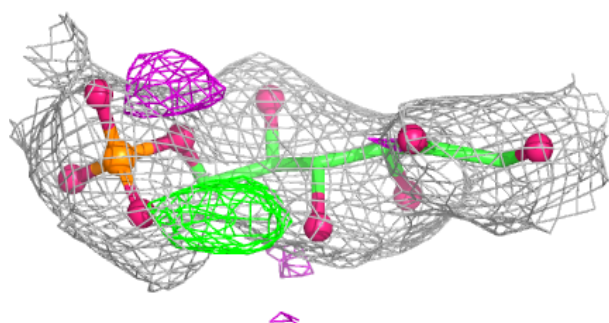
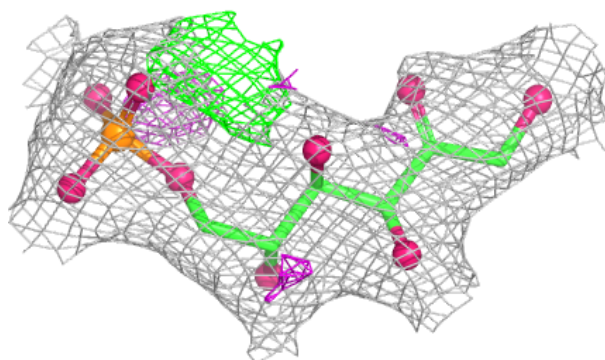
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	F6R	B	800	16/16	0.86	0.14	44,48,51,52	0
2	F6R	A	800	16/16	0.91	0.11	38,40,41,41	0
3	CL	C	1691	1/1	0.95	0.07	45,45,45,45	0
2	F6R	D	800	16/16	0.96	0.08	28,30,32,33	0
2	F6R	C	800	16/16	0.97	0.07	29,31,33,34	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

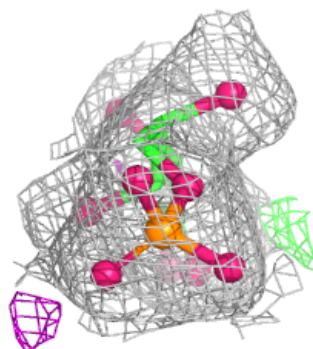
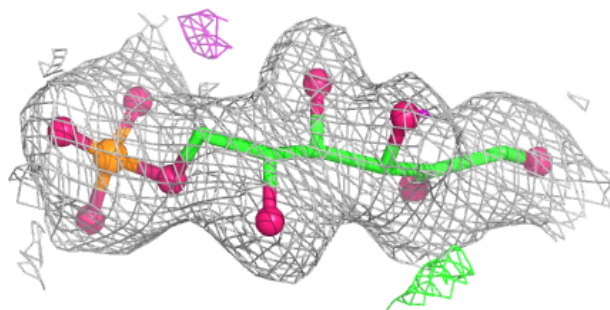
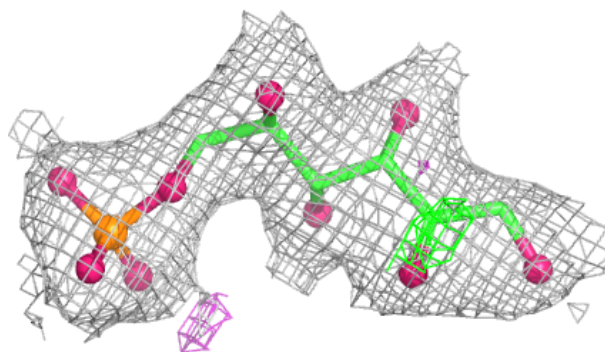
Electron density around F6R B 800:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around F6R D 800:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.